DRUGLIKENESS PREDICTION AND IN-SILICO ANTI-ANXIETY ACTIVITY TESTING ON GABA RECEPTORS AND ROLL ON AROMATHERAPY PREPARATION FROM Lavandula angustifolia ESSENTIAL OIL

Ferry Ranko Soegiarto*, Azminah, Roisah Nawatila

***Corresponding author:** ferrysoegiarto23@gmail.com

Abstact

Anxiety is an anxiety disorder that will experience excessive fear. Anti-anxiety therapy generally uses benzodiazepine drug therapy as a sedative-hypnotic drug that binds to chloride ion channels at the GABA receptor. In addition to drug therapy, complementary therapies can be used, namely aromatherapy. Aromatherapy from Lavandula angustifolia essential oil has benefits as an anti-anxiety therapy. Aromatherapy has many dosage forms so it is necessary to develop a stable dosage form, namely roll on. This study aims to determine the prediction of druglikeness and activity of the essential oil compound Lavandula angustifolia in silico using the molecular docking method for the GABA PDB receptor code 6X3X using Autodock Vina. The results showed that there were 28 compounds that met druglikeness and there were 4 compounds with a bond interaction suitability of 57%. Continued development of roll-on aromatherapy preparations with different types of carrier oil. The results showed that there were differences in preparations using carrier oil olive oil on viscosity parameters, but all preparations were stable on organoleptic parameters, pH and homogeneity for 1 month.

Keyword: *Anxiety, GABA, Lavandula angustifolia*, *aromatherapy, roll on*

1. Introduction

Anxiety is one of the most common psychological disorders in the world. Anxiety is a defensive reaction to protect yourself from more severe emotional mental disorders (Murticwidayanti and Ikawati, 2021). Anxiety can be overcome with pharmacological treatment such as benzodiazepines which can also be used as anti-anxiety therapy; however, the use of benzodiazepines can cause drug dependence (Craske and Stein, 2016; Penninx et al., 2021). $GABA_A$ (Gamma (γ)-aminobutyric acid) receptors are receptors responsible for targeting anti-anxiety drugs. Benzodiazepines work by binding to $GABA_A$ receptors which activate complex, ligand gated chloride channels to increase the entry of chloride ions into neurons and cause hyperpolarization (Kalueff and Nutt, 2007; Sankar, 2012; Kim, 2020)

Aromatherapy uses essential oils as the main ingredient extracted from plant parts such as flowers, leaves, stems, fruit, roots, and resin. The use of this essential oil as an alternative medicine that can reduce anxiety and is proven to avoid side effects caused using chronic anti-anxiety drugs and synthetic antidepressants (Lizarraga-Valderrama,2021). Lavender or Lavandula angustifolia, is an herbal plant that comes from the Lamiaceae family. This plant is native to the Mediterranean region and has grown worldwide due to the high market price for Lavandula angustifolia essential oil. This essential oil is widely used as perfume, soap, food flavoring, lotion, and aromatherapy.

The use of aromatherapy preparations is a therapeutic action using essential oils which are useful for improving a person's physical and psychological condition for the better (Fatmawati, 2022). Roll on preparations are used to improve the well-being of the body, mind, and spirit. In addition, roll on preparations are also the most widely used aromatherapy preparations. Besides being easy to use, interesting and unique, this preparation can relieve aches, dizziness, headaches, and other conditions (Sofiani and Pratiwi, 2017). Another advantage of roll on aromatherapy preparations is that their use is carried out by inhalation which is the most widely used and effective route in aromatherapy preparations. (Farrar and Farrar, 2020).

In-silico testing is a rapidly growing method that globally includes the development of techniques using software to capture, analyze, and integrate biological and medical data from multiple sources. Specifically, in-silico testing defines the use of this information in the creation of computational or simulation models that can be used to make predictions, suggest hypotheses, and ultimately provide discoveries or advances in medicine and therapy (Ekins, Mestres and Testa, 2007). Molecular Docking is a key tool in structural molecular biology and computer-assisted drug design. The goal of ligand-protein docking is to predict the dominant binding mode of a ligand with a protein whose three-dimensional structure is known (Morris and Lim-Wilby, 2008).

Based on the above problems, a molecular docking analysis of Lavandula angustifolia essential oil was carried out using the AutoDock Vina program to determine anantiolytic activity at the GABA receptor (PDB Code 6X3X) and druglikeness prediction was carried out using swissADME and Molsoft's online web. Furthermore, another alternative was made from the form of aromatherapy preparations in the form of roll-on preparations using various types of carrier oil, namely olive oil (Formula 1), combination of olive oil-triglyceride caprate (Formula 2), and combination olive oil-VCO (Formula 3). Analysis of druglikeness prediction data was processed using radar diagrams, bars, and two-dimensional graphs while for the results of evaluation data on the physical characteristics of roll on preparations, it was analyzed using the one way ANOVA method.

2. Method

Free Variables

The independent variables in this study were the parameters of the physicochemical properties of the essential oil compound Lavandula angustifolia , the concentration of carrier oil such as olive oil as much as 94.9% in Formula 1, the combination of olive oil and caprylate as much as 20-79.5% in Formula 2, and the combination of olive oil and VCO as much as 20-74.9% in Formula 3.

Dependent Variable
The dependent variables in this study were the parameter druglikeness and activity test of Lavandula angustifolia essential oil in-silico. Test parameters for evaluating the physico-chemical characteristics of roll on aromatherapy preparations which include organoleptic tests, pH tests, irritation tests, homogeneity tests, and viscosity tests.

Controlled Variables
The controlled variables in this study were the concentration of the active ingredient Lavandula angustifolia essential oil (5%), the type of additive (BHT), the procedure for making aromatherapy therapeutic roll on, the conditions of manufacture and storage.

Research Tools
The In-silico research tools in this study were laptops, PubChem, MarvinSketch, swis-sADME, BIOVIA Discovery Studio Visualizer 2021, AutoDock Vina 1.1.2, and AutoDock Tools 1.5.7. The tools used for the manufacture of roll on aromatherapy preparations are in the form of a magnetic stirrer, cover glass, object glass, beaker glass, analytical balance, Brookfield Cone and Plate viscometer, universal indicator, measuring cup, pipette, spatula, parchment paper, watch glass, spoon horns, and roll on bottles,

Research Materials
The In-silico research material in this study was a database of compounds from Lavandula angustifolia essential oil and the target receptor, namely the GABA receptor (PDB Code: 6X3X), with a 3D structure that can be viewed using the RSCB Protein Data Bank (PDB) website. The materials used for the manufacture of roll on aromatherapy preparations are Lavandula an-gustifolia essential oil, olive oil, Virgin Coconut Oil (VCO), caprylic triglyceride (caprate), and butyl hydroxy toluene (BHT).

Collection of Compound Database
Compounds from the essential oil of Lavandula angustifolia were collected using the PubMed data base and obtained 62 compounds (Smigielski et al., 2009)

Druglikeness Parameter Analysis
Druglikeness parameter analysis of compounds from Lavandula angustifolia essential oil was carried out by entering the SMILES (*.SMILES) structure of the compound in the swissADME web-based tool (http://www.swissadme.ch/) to obtain MLOGP, HBA, HBD, and MLOGP data. MW.

Molecular docking program validation
The program used for molecular docking is AutoDock Vina 1.1.2. Next, the re-docking results were visualized using the BIOVIA Discovery Studio Visualizer 2021. The validation parameters observed were the RMSD (Root Mean Square Deviation) value between the original ligand and the re-docked ligand.

Molecular docking
Molecular Docking in this study was carried out using the Auto-Dock Vina 1.1.2 program. Interaction and visualization of molecular docking of Lavandula an-gustifolia essential oil compounds with GABA receptors using the BIOVIA Discovery Studio Visualizer 2021 program to visualize bond interactions (hydrogen bonds and hydrophobic interactions) in 2D and 3D

Design of Aromatherapy Roll on Formula

Table 1. Design of Aromatherapy roll on formulation

Bahan	Function	Concentration (%)			Lab scale amount (100 mL)
		F1	F2	F3	
Lavandula angustifolia essential oil	Active ingredients	5 %	5 %	5 %	5 mL
BHT	Antioxidant	0,1 %	0,1 %	0,1 %	0,1 g
Olive Oil	Carrier Oil	Ad 100 %	20 %	20 %	20 mL
Caprylic triglyceride	Carrier Oil	-	Ad 100 %	-	Ad 100 %
VCO	Carrier Oil	-	-	Ad 100 %	

Making Aromatherapy roll on preparations

Prepare the necessary tools and materials. Then calibrate a 10 mL roll on bottle. Then, 5 mL of Lavandula angustifolia essential oil was measured using a measuring cup and calibrating a 20 mL beaker glass and adding olive oil to the limit of the calibration mark. After that, weigh 0.1 gram of BHT using parchment paper. Then, put the olive oil into a 100 mL beaker glass, then add BHT and then cover the top of the beaker glass using aluminum foil. Stir the above using a magnetic stirrer until dissolved at room temperature. Then add Lavandula angustifolia essential oil to the above mixture then cover again with aluminum foil and stir again using a magnetic stirrer until homogeneous. After everything is mixed homogeneously, add carrier oil to the limit of 100 mL, then cover the beaker glass and stir on a magnetic stirrer. The finished essential oil is put into a calibrated 10 mL roll on bottle. Then, put it into the aromatherapy roll on packaging. Follow the same method of preparation with a different carrier oil.

Physico-chemical characteristics of aromatherapy roll on.

a. Organoleptic test

Organoleptic tests observed included shape, color, and smell of roll on aromatherapy preparations. This test was carried out visually using on day 0, day 7, day 14, day 21, and day 28 (Nurcahyo and Riyanta, 2019)

b. Test the pH.

The pH test was carried out by dipping universal paper in the roll on aromatherapy preparation and then comparing it to the standard pH color. The pH of the preparation can be said to be good where a preparation has a range that corresponds to the pH of the skin, namely 4.5-6.5. pH testing was carried out on day 0, day 7, day 14, day 21, and day 28 (Fatmawati, 2022)

c. Homogeneity test

The homogeneity test was carried out by placing a few drops of the preparation on an object glass, then flattening it with the help of a cover glass. It will be seen visually whether there are impurities or not. Preparations can be said to be homogeneous if no impurities are seen in the preparation. pH testing was carried out on day 0, day 7, day 14, day 21, and day 28 (Nurcahyo and Riyanta, 2019)

d. Irritation Test

This test is carried out by applying the preparation on the surface of the skin and then leaving it for up to 15 minutes to see the effect of the preparation on the skin. If there is no rash, itching, burning and swelling on the skin, the preparation is said to be safe for use because it does not cause any irritating effects. Irritation test was carried out on day 14, day 21, and day 28 (Nurcahyo and Riyanta, 2019)

e. Viscosity Test

Viscosity was checked using a Brookfield viscometer of the Cone and Plate DV-I type. Remove the sample cup from the apparatus. The sample is placed in the sample cup, making sure the sample is free of bubbles and evenly distributed on the surface of the cup. Reattach the sample cup to the viscometer, turn on the viscometer, then allow a few moments for the reading to stabilize. Record the viscosity reading on the display. Viscosity tests were carried out on day 0, day 7, day 14, day 21, and day 28 by doing 3 replications (Fitriani et al., 2016)

3. Results

Results of Druglikeness Parameter Analysis

The results of the druglikeness parameter analysis of compounds from Lavandula angustifolia essential oil according to Lipinski using SwissADME web-based tools

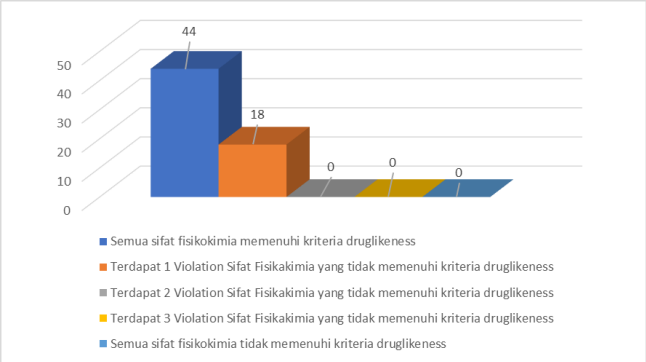

Figure 1 Analysis of Druglikeness Parameters of Compounds in Lavandula angustifolia Essential Oil according to Lipinski using a bar chart for the number of compounds that meet Drug-likeness parameters according to Lipinski.

Molecular Docking Program Validation Results

Results of validation of the molecular docking program for GABA receptors (PDB code: 6X3X) using AutoDock Vina 1.1.2. and the validation parameter is the RMSD (Root Mean Square Deviation) value obtained using the BIOVIA Discovery Studio Visualizer 2021 program. For the GABA Receptor, a ligand is used, namely DZP with a gridbox size of 18 x 18 x 18 and gridcenter x (145,574), y (123,299), z (122,487). The RMSD value obtained from the GABA Receptor validation results is 0.6633 Å and the bond energy value is -9.5 kcal/mol.

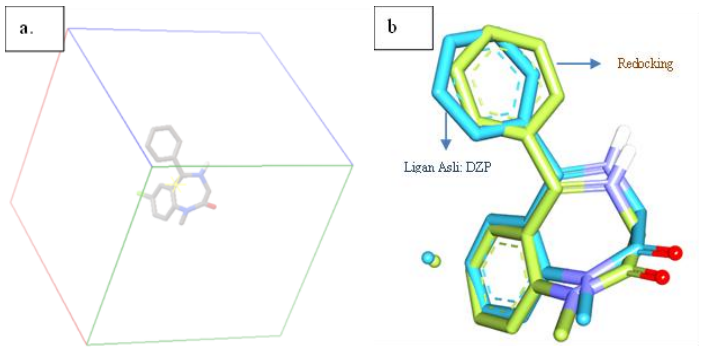

Figure 2. Molecular Docking Program Validation a. GABA Receptor Gridbox with DZP Native Ligand, b. Visualization of Original Ligand Structure (blue) and Redocking Result Ligand (green)

Molecular docking results

Molecular docking between Lavandula angustifolia compounds and receptor targets was carried out using the AutoDock Vina 1.1.2 program. The results of molecular docking obtained activity predictions in the form of bond energy (kcal/mol). The results of the visualization of the molecular docking structure of the essential oil compound Lavandula angustifolia with the receptor cause the interaction of hydrophobic bonds, hydrogen bonds and other bonds. The interaction results consist of variants and positions of amino acid residues and types of bonds obtained using the BIOVIA Discovery Studio Visualizer 2021 program.

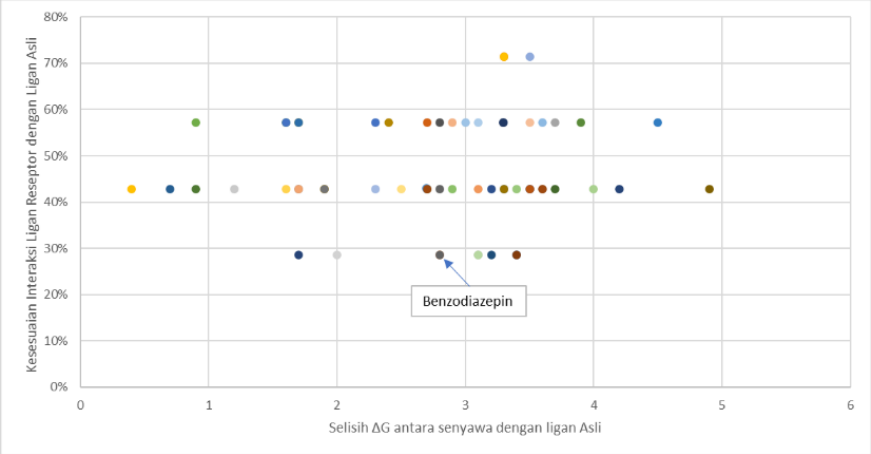

Figure 3. Two-dimensional graph of the relationship between the difference in ΔG of the compound and the original ligand to the percentage of conformity of the interaction between the receptor ligand and the original ligand

Organoleptic Test Results

Organoleptic testing for F1, F2, and F3 was carried out from day 0 to day 28. Parameters observed were shape, color, and smell. The organoleptic test results of Roll On Aromatherapy Preparations on Observation Day 0 to Day 28 had the same results on F1, F2, and F3. F1 is in the form of a clear, yellow solution with a characteristic lavender odor. F2 and F3 are in the form of a clear, pale yellow solution with a characteristic lavender odor

pH Test Results

pH testing on F1, F2, and F3 was carried out from day 0 to day 28. In this study using a universal indicator to determine a preparation in an acidic or alkaline environment. Based on the results of pH measurements using a universal indicator, it showed pH = 5 in all roll on aromatherapy formulations from day 0 to day 28.

Homogeneity Test Results

Homogeneity tests on F1, F2, and F3 were carried out from day 0 to day 28. This test is carried out by placing a few drops of the roll on aromatherapy preparation on an object glass, then flattening it with the help of a cover glass. The purpose of the homogeneity test is to visually see whether the roll on aromatherapy preparations contain impurities or not. Preparations can be said to be homogeneous if no impurities are seen in the preparation. Based on the homogeneity test results of Roll On Aromatherapy Preparations on Observation Day 0 to Day 28, the results were homogeneous, there were no impurities on F1, F2, and F3.

Irritation Test Results

Irritation Testing on F1, F2, and F3 was carried out on day 14 to day 28. The irritation test was carried out on 10 panelists by applying a small amount of the preparation on the skin surface and then letting it sit for up to 15 minutes. The purpose of this test is to see whether roll on aromatherapy preparations are safe to use or can cause rashes, itching, burning, and swelling of

the skin. Based on the Irritation test on F1, F2, and F3 carried out on day 14 to day 28, the preparation did not cause rashes, itching, burning, and swelling of the skin.

Viscosity Test Results

Viscosity testing on F1, F2, and F3 was carried out from day 0 to day 28. Viscosity was observed using a Cone and Plate DV-I Brookfield viscometer on spindle 41 and readings were taken at 100 rpm. Based on the results of the viscosity test of Lavandula angustifolia roll on aromatherapy preparations from Day 0 to Day 28, all preparations had Newtonian flow properties.

4. Discussion

An analysis of druglikeness parameters was carried out using Lipinski's Fifth Law (Rule of Five) which states that a compound has poor absorption and permeability if there are 2 parameters outside the specified range (violation). Parameters are meant if the molecule is ≥ 500, has a logP value ≥ 5 (or MlogP ≥ 4.15), has ≥ 5 HBD , and has ≥ 10 HBA (Lipinski et al., 2001). In this study, Lipinski's druglikeness parameter data was obtained using the SwissADME web-based tool.

Data from the analysis of druglikeness parameters according to Lipinski can be seen in Figure 1 which is a bar chart showing the number of compounds that meet the druglikeness parameters according to Lipinski, where 44 compounds meet the druglikeness criteria in all four parameters and 18 compounds have 1 violation in one of the parameters druglikeness that is MlogP. These compounds are (E)-β-Farnesene (4.84), Cadalene (5.62), Camphene (4.29), 3-Carene (4.29), Germecrene D (4.53), Sabinene (4 ,29), trans-Calamenene (5,45), α-Bergamotene (4,63), α-Curcumene (5,75), α-Caryophyllene (4,53), α-Pinene (4,29), α -Santalene (5,65), α-Thujene (4,29), β-Caryophyllene (4,63), β-Cymene (4,47), γ-Cadinene (4,63), δ-Cadinene (4, 63), and ρ-Cymene (4,47).

The next stage was to analyze the activity of compounds from Lavandula an-gustifolia essential oil to obtain parameters of bond energies and bond interactions (hydrogen bonds and hydrophobic interactions). The activity of a drug occurs due to the interaction of the drug molecule with the functional group of the receptor molecule. Drug-receptor interactions can take place due to the strength of certain chemical bonds. In general, drug-receptor binding is reversible so that the drug leaves the receptor if levels outside the cell decrease. Compounds can combine several weak bonds to produce bonds that are strong and stable enough, whereas for longer and irreversible bonds, stronger bonds such as covalent bonds are needed. Chemical bonds that are often found in drug-receptor interactions include covalent bonds, ionic bonds, hydrogen bonds, ion-dipole bonds, dipole-dipole bonds, charge transfer, Van der Waals bonds, and hydrophobic bonds (Siswandono, 2016)

Figure 3 shows the results of the activity parameters of compounds from Lavandula angustifolia essential oil on GABA receptors (6X3X) with a bond energy DZP value of -9.5 kcal/mol. Meanwhile, benzodiazepines as a GABA receptor comparator drug have a binding energy of -6.7 kcal/mol. 62 Compounds in Lavandula angustifolia essential oil have a binding energy range at GABA receptors between -9.1 kcal/mol and -5 kcal/mol, with 28 compounds in having a better energy value than the comparator drug (-6.7). These compounds are (E)-β-Farnesene (-7,2), 1-epi-Cubenol (-7,9), Bornyl acetate (-6,7), Cadalene (-8,8), Caryophyllene oxide (- 7,8), Geranyl acetate (-6,8), Germacrene D (-7,8), Globulol (-7,6), Leden Oxide II (-8,3), Ledol (-7,6), Neryl acetate (-6,7), Piperitone (-6,8), t-Cadinol (-7,8), trans-Calamenene (-7,9), trans-Sesquisabinene hydrate (-7,6), α-Bergamotene (-7,1), α-Cadinol (-7,8), α-Curcumene (-8,6), α-Caryophy llene (-7,2), α-Santalene (-7,5), α- Terpinolene (-7), β-Caryophyllene (-7,9), β-Cymene (-6,7), γ-Cadinene (-9,1), γ-Terpinene (-6,8), δ-Cadinene (-8.6), δ-Cadinol (-7.8), and ρ-Cymene (-6.8).

After the in-silico test, the roll-on aromatherapy formulation was carried out using 5% Lavandula angustifolia essential oil, different carrier oils, namely olive oil (F1), Caprate Triglycerides (F2), and Virgin Coconut Oil (F3). . Then added additional ingredients such as BHT. Each roll on aromatherapy preparation will be subjected to physico-chemical characterization which includes organoleptic tests, pH tests, homogeneity tests, irritation tests, and viscosity tests. After that, stability is observed for 1 month (0th day, 7th day, 14th day, 21st day, and 28th day)

on organoleptic test parameters, pH test, homogeneity test, and viscosity test. Meanwhile, the irritation test was carried out for 2 weeks (14th day, 21st day, 28th day).

Organoleptic observations were carried out descriptively using the five human senses in each roll on aromatherapy preparation, namely using carrier oil olive oil (F1), caprylic triglycerides (F2), VCO (F3). Parameters observed in organoleptic include shape, odor, and color of the preparation. Before storage, all of the oils showed a shape that was not much different between the three oil formulas, for the color it had a yellow to pale yellow color, while for the smell it had a characteristic lavender smell. Essential oils with carrier oil olive oil (F1) have a yellow color with a characteristic lavender aroma, essential oils with caprylic triglyceride (F2) carrier oil have a pale yellow color with a characteristic lavender aroma, and essential oils with VCO carrier oil (F3) has a pale yellow color with a characteristic lavender odor. After being stored for 1 month, all roll on aromatherapy preparations showed no change in color and odor before storage.

The next step was to observe the pH test which was carried out descriptively using a universal indicator dipped in each roll on aromatherapy preparation. The results of the pH test showed that the three roll on aromatherapy preparations on La-vandula angustifolia essential oil with carrier oil, olive oil (F1), caprylic triglyceride (F2), and VCO (F3) had the same pH value before and after storage for 1 month, namely 5. Based on the pH test parameters, the preparation can be said to be stable during storage because there is no change in pH. The pH results of the preparation can be said to be safe for the skin, and meet the pH requirements of topical preparations, namely 4.5-6.5. The suitability of the pH of topical preparations will affect acidity or alkalinity so that the skin does not experience irritation (Fatmawati, 2022).

Observations on the homogeneity test were carried out descriptively. This test was carried out by placing a few drops of roll on aromatherapy preparations, namely Lavandula an-gustifolia essential oil with carrier oil, olive oil (F1), caprylic triglyceride (F2), and VCO (F3) on an object glass and then leveling it with the help of a cover glass. The purpose of the homogeneity test was to see whether all the ingredients in the roll on aromatherapy formulation were mixed perfectly in the preparation. The results of the homogeneity test observations showed that all preparations were homogeneous with marked absence of impurities on the surface of the object glass for 1 month. Based on the homogeneity test parameters, the preparation can be said to be homogeneous during storage because no impurities are visible (Nurcahyo and Riyanta, 2019).

Observations on the irritation test were carried out descriptively. This test was carried out on 10 panelists with evidence of a consent form signed by the respondent. A small amount of roll on aromatherapy preparation, namely Lavandula angustifolia essential oil with carrier oil, olive oil (F1), caprylic triglyceride (F2), and VCO (F3) is rubbed on the surface of the skin and then left for 15 minutes and the results showed no rashes, itching, sore, and swollen so that it can be said that roll on aromatherapy preparations can be said to be safe because they do not cause irritating effects (Nurcahyo and Riyanta, 2019).

Viscosity test observations are carried out with the aim of seeing the viscosity of a preparation. Analysis of the viscosity test results for roll on aromatherapy preparations, namely Lavandula angustifolia essential oil with carrier oil, olive oil (F1), caprylic triglyceride (F2), and VCO (F3) was carried out using One Way Anova to determine the P value obtained whether there was an effect or no effect. There were 8 results of data analysis, namely comparing F1, F2, and F3 on day 0 to day 28, comparing F1 on day 0 to day 28, comparing F2 on day 0 to day 3. 28, and compared F2 on day 0 to day 28.

Based on the 8 results of data analysis using One Way Anova, F1, F2, and F3 on day 0 to day 28 were obtained with a value of $P = <0.001$ ($P <0.05$), which means there was a significant difference. Then the results of One Way Anova show that F1 from day 0 to day 28 was obtained with a value of $P = 0.04$, F2 from day 0 to day 28 was obtained with a value of $P = 0.735$, and F3 on day -0 until the 28th day was obtained with a value of $P = 0.1$. These results show that in F2 and F3 it is said that there is no significant difference in the two formulas while in F1 it is said that there is a significant difference so that the preparation in F1 is said to be unstable.

There was a significant difference in the F1 preparation indicating that the analysis of the results of the viscosity test of the roll on aromatherapy preparation, namely Lavandula angustifolia essential oil with carrier oil, olive oil was said to be unstable. Viscosity instability is due to differences in temperature at the time of manufacture and temperature at the time of storage.

Viscosity is inversely proportional to temperature, meaning that if there is an increase in temperature, the viscosity will decrease and if there is a decrease in temperature, the viscosity will increase (Peri, 2014)

Observations of this viscosity test also saw the flow properties of roll on aromatherapy preparations, namely Lavandula angustifolia essential oil with carrier oil olive oil (F1), caprylic triglyceride (F2), and VCO (F3) on day 0 to day 28 showed that the flow of roll on aromatherapy preparations namely Lavandula angustifolia essential oil in F1, F2, and F3 is said to have Newtonian flow properties. The results of the flow properties in F1 are supported by research (Ashqer, Bahti and Musameh, 2014) saying that the results of viscosity measurements show that olive oil has a flow index value close to 1. The results of the flow properties of F2 are supported by research (Geller and Goodrum, 2000) saying that caprylic triglyceride has a flow transition from non-Newtonian to Newtonian. The results of the flow properties at F3 are supported by research (Tipvarakarnkoon, Blochwitz and Senge, 2008) which states that the flow properties of VCO have Newtonian flow properties.

5. Conclusion

From this study it can be predicted that the essential oil compound Lavandula angustifolia has activity against GABA receptors so that it can be used as a complementary therapy in anti-anxiety therapy. Then, a more stable preparation was developed from Lavandula angustifolia essential oil in roll on form. From the production of roll on aromatherapy preparations with Lavandula angustifolia essential oil, it can be said that preparations using caprylic triglyceride (F2) and VCO (F3) carrier oils are better than using olive oil (F1) carrier oil due to the instability of the preparation in terms of viscosity. Besides that, roll on aromatherapy preparations with Lavandula angustifolia essential oil can be said to be safe to use because they do not cause irritation. Further research is needed on the essential oil compounds of Lavandula angustifolia by knowing the ADME parameters and the compound's toxicity. In addition, the essential oil compound Lavandula angustifolia which meets the parameters of drug likeness and activity as an anti-anxiety can be isolated and carried out further research in vivo and in vitro.

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ABSTRACT AO8

DRUG-LIKENESS PREDICTION AND SLEEP DISORDER ACTIVITY TEST (IN SILICO) OF BASIL ESSENTIAL OIL AND ITS FORMULATION INTO AROMATHERAPY DERMA STICKS

Rahayu[1], Azminah[2], Roisah Nawatila[3*]

[1]*Faculty of Pharmacy, University of Surabaya, Indonesia*
[2]*Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Surabaya, Indonesia*
[3]*Department of Pharmaceutics, Faculty of Pharmacy, University of Surabaya, Indonesia*

*) Corresponding author: roisah@staff.ubaya.ac.id

Background:

Sleep disorder is a manifestation of mental health problems. Sleep disorder therapy usually uses a benzodiazepine class that acts on the therapeutic target of $GABA_A$ receptors. The use of drug therapy for sleep disorders can be complemented by aromatherapy to support the healing process. Aromatherapy from basil essential oil has benefits as a sleep disorder therapy. This aromatherapy needed to be developed into derma sticks that are more stable and more effective to use.

Methods:

This study aims to determine the prediction of drug-likeness and activity of compounds basil essential oil by molecular docking method in silico against the $GABA_A$ PDB receptor code 6D6T using *Autodock Vina* program. After that, the research will continue to develop the basil essential oil into aromatherapy derma sticks by determining the effect of different concentration of stearyl alcohol as hard agent in F1, F2, and F3 (20%, 25%, and 30%, respectively) on the physical characteristics (organoleptic, melting point, homogeneity, hardness, comfort test) and derma sticks stability (days 0, 7, 14, and 28).

Results:

The results of molecular docking showed that there were 4 compounds that met drug-likeness and there was 1 compound with a bond interaction suitability of 63%. The results showed that the higher concentration of stearyl alcohol, the better physical characteristics. In addition, all formulas provide good experience and comfort to use when applied by respondents. All formulas showed good physical stability results on days 0, 7, 14, 28.

Conclusions:

66% of basil essential oil compounds or 51 compounds out of 75 compounds meet the drug likeness criteria according to Lipinski's Law 5 for drug

similarity. The activity prediction showed 63% of basil essential oil compounds are better than the comparator drug. Additionally, variations concentration in stearyl alcohol as hard agents can affect the physical characteristics of aromatherapy derma sticks preparation.

Keywords: Sleep Disorder, Aromatherapy, Basil, In Silico, Derma Sticks

ABSTRACT BOOK

ICSM 2023

International Conference and Scientific Meeting

Department of Pharmacy, Faculty of Medicine,
Brawijaya University

ICSM 2023

INTERNATIONAL CONFERENCE AND SCIENTIFIC MEETING

ABSTRACT BOOK

Department of Pharmacy, Faculty of Medicine, Brawijaya University

OPENING REMARKS

DEAN OF FACULTY OF MEDICINE, BRAWIJAYA UNIVERSITY

Dear distinguished speakers, esteemed participants and members of the Faculty of Medicine, Universitas Brawijaya.

Good morning

I am delighted to stand before you as the representative of our solid organising committee, which has put so much effort over the past four months, culminating in this special scientific event called the first International Conference and Scientific Meeting (ICSM) 2023.

I hope that ICSM 2023 will provide y10ou with an excellent opportunity to disseminate your research and enhance your scientific performance by networking with the international scientific community, while learning about groundbreaking research and the latest practice-changing innovations.

This year, the ICSM Spotlight will be dedicated to a topic relevant to current health sciences and drug development. I encourage you to take this opportunity to learn about important updates in medical, biomedical, pharmaceutical, pharmacological and midwifery research that will be presented later.

I wish this event every success and hope that it can continue as an annual scientific event.

I am also pleased to inform all participants that selected articles from this event will be published in reputable journals, including a Scopus-indexed journal with which we have been in contact, following a peer-review process, of course.

I would like to express my sincere gratitude to the organising committee, the generous sponsors and all the distinguished speakers who are willing to contribute to this event.

Let's join forces with our colleagues and immerse ourselves in the excitement and energy of the first International Conference and Scientific Meeting 2023.

Thank you

OPENING REMARKS

CHAIRMAN OF THE INTERNATIONAL CONFERENCE AND SCIENTIFIC MEETING (ICSM) 2023

Assalamu'alaikum Wr. Wb., Shalom, Om Swastiastu, Namo Budaya, Salam Kebajikan, Selamat Sejahtera for all of you.

Honourable, Rector of Universitas Brawijaya, Dean of Medical Faculty, Universitas Brawijaya, distinguished speakers, and all participants.

First of all, I would like to say a big thank you for your presence at this event. Your participation is a proof of extraordinary support for us in organizing this international seminar. The International Conference and Scientific Meeting (ICSM 2023) with the theme of "Scientific Meeting in Current Health Sciences and Drug Development" is an event organized by the Department of Pharmacy with contributions from the Department of Medicine and Midwifery, Faculty of Medicine, Brawijaya University. This event is participated by leading academic scientists, researchers and practitioners from Indonesia and other countries, both online and offline, to exchange experience and research findings in most aspecst of drug development and health sciences.

Invited speakers in this conference come from various countries, such as Italy, Taiwan, Japan, Czech Republic, Brunei Darussalam and Indonesia. Topics presented include disease therapy, vaccines, metabolomic analysis, drug discovery in herbs, nano-sized particles, pharmacology, biomedicine, and pregnancy management. The speakers exhibit their expertise and competence in the field of research or practice that had been carried out.
The aim of ICSM 2023 is to enrich insights especially in health sciences, that have now entered the era of society 5.0. In the era of society 5.0, there is a merger between cyberspace and physical space (the real world). All research and health service data results are stored and analyzed via AI (Artificial Intelligence). So that Current Health Sciences is developed more human-centered. Through this event, we hope that practical and dynamic health innovations will emerge following developments in science based on human needs.

This conference is the real contribution of the Faculty of Medicine, Brawijaya University to the development of research and health services. Our hope is that this seminar will become a forum for sharing knowledge that can give birth to new breakthroughs in health sciences.
I thank all those who have contributed. Thank you to the speakers who were willing to attend, to the committee who have worked hard to prepare ICSM 2023, and thank you to all the attendees. I apologize for any shortcoming in organizing this event.

Thank you so much.

Wassalamualaikum Wr Wb.

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THE INTERNATIONAL CONFERENCE AND SCIENTIFIC MEETING (ICSM) 2023
Atria Hotel Malang, November 4th 2023

Link Zoom Meeting :
s.ub.ac.id/icsm2023

Time	Agenda	
07.30 – 08.00	Registration (Offline – Online Zoom Meeting)	
08.00 – 08.30	Opening Ceremony 1. Traditional Dance "Jejer Gandrung Banyuwangi" 2. Welcome speech from Chairperson of ICSM 2023 (Dr. apt. Anisyah Achmad, S.Si., Sp.FRS) 3. Speech from Rector UB (Prof. Widodo, S.Si., M.Si., Ph.D.Med.Sc)	
08.30 – 09.15	**Plenary Speaker 1** Prof. Salvatore Di Somma, MD, Ph.D. (Sapienza University of Rome, Italy) Topic: Multidisciplinary Practical Guidance for Acute Heart Failure	
09.15 – 10.00	**Plenary Speaker 2** Prof. Tetsuya Ozeki (Nagoya City University) Topic: Novel Targeted Therapeutic Nano-sized Particles	
10.00 – 10.15	Q and A (Discussion)	
10.15 – 10.30	Coffee Break and Parallel Session Preparation	
10.30 – 11.10	**Parallel Session 1**	**Parallel Session 2**
10.30 – 11.10	Prof. Shawn Chen Hsiang-Yin, Pharm.D., Taipei Medical University Topic: Machine Learning Application for Pharmacy Service (ONLINE)	apt. Neni Nuraini, S.Si, PT Biofarma Indonesia Topic: Vaccine Bioprocess Development and Challenges in Indonesia (ONLINE)
11.10 – 11.50	Dr Siti Rohaiza Ahmad, Universiti Brunei Darussalam Topic: Recent issues in the management of anaemia in pregnancy (ONLINE)	Prof. Dr. apt. Abdul Rohman, S.F., M.Si., Faculty of Pharmacy, UGM Topic: Metabolomic study on drug development and analysis (OFFLINE)
11.50 – 12.30	(Kathryn) Louise Walker, University of Nottingham Topic: Zinc and Vit D supplementation during pregnancy (ONLINE)	Prof. Ing. Lucie Cahlíková, Ph.D., Faculty of Pharmacy in Hradec Kralove, Charles University, Czech Republic Topic: Drug discovery from herbals: An Integrated Approach (OFFLINE)
12.30 – 12.50	Q and A (Discussion)	Q and A (Discussion)
12.50 – 13.40	Lunch Break	
13.40 – 15.00	Poster Presentation and Oral Presentation Session 1*	
15.00 – 15.15	Coffee break and parallel session preparation	
15.15 – 16.15	Oral Presentation Session 2*	
16.15 – 16.45	Oral and Poster Award	
17.00	Closing	

*The attachment can be seen below

POSTER PRESENTER SCHEDULE
Saturday, November 4th 2023
Presentation Session: 13.40 – 15.00

CODE	NAME OF POSTER PRESENTATION	ABSTRACT TITLE
AP1	Lestyo Wulandari	Determination of Moisture Content of Cinnamon Bark Powder (Cinnamomum Burmanii Nees &Amp, T.Nees) Using Nir Spectroscopy And Chemometric
AP2	Nafisah Aulia Ramadhani	A Screening Method Based On Spectroscopy Ftir and Chemometrics To Identify Adulterated Chili Powder With Red Textiles Dyes
AP3	Syahril Maulid Dia	Fourier Transform Infrared Spectroscopy And Chemometrics For Screening The Adulteration on Turmeric Powder With Yellow Textiles Dyes
AP4	Laffael Kevin Immanuel	Application of Box–Behnken Design Combined Response Surface Methodology to Optimize Hplc for Quantifying Paracetamol in Jamu Pegal Linu
AP5	Lia Puspitasari	Validation of Isoniazid Analysis Method in 2 Fixed-Dosed Combination Dispersible Tablets by High-Performance Liquid Chromatography
AP6	Ferry Ranko Soegiarto	Drug-Likeness Prediction And Anti-Anxiety Activity Test (In Silico) of Lavandula Angustifolia Essential Oil and Its Formulation Into Aromatherapy Roll-On
AP7	Nia Kristiningrum	Determination of Total Phenolic Content in Capsule Preparation of Garlic Extract (Allium Sativum, L.) by Nir-Chemometric Method
AP8	Ni Komang Tri Widya Putri	The Application of Box-Behnken Design in The Optimization of Hplc For Quantifying Paracetamol in Jamu Asam Urat
AP9	Indah Purnama Sary	Molecularly Imprinted Polymer for Capturing Quercetin From Allium Cepa L.
AP10	Dian Agung Pangaribowo	Design, Synthesis, Antiproliferative Activity, and Molecular Docking Studies of Novel Cinnamic Acid-Indoline Derivatives as Anticancer Agents
BP1	Alina Chusna Yain	Systematic Literature Review: The Use Of Traditional Medicines For The Prevention and Companion of The Treatment of Covid-19
BP2	Salsabilah Aida Fitri	Systematic Literature Review: Pharmacists' Knowledge And Appropriateness of Recommendations For The Treatment of Pediatric Diarrhea
BP3	Rindha Agata Fauzia	Knowledge and Attitude Regarding Moisturizer Use in Malang: A Cross-Sectional, Survey-Based Study
BP4	Ema Pristi Yunita	Analysis of Sociodemographic Factors, Blood Pressure Categories, and Anti-Hypertensive Medication on Patient Adherence to Anti-Hypertensive Medication (A Study At Sakinah Islamic Hospital, Mojokerto District, Indonesia)
CP1	Bunga Prihardina	Immunomodulatory Potential of Water Extract of Benalu Batu Stem (Begonia Medicinalis)

CP2	Achmad Gigih Andy Putra	Pharmacological Potential Of Moringa Oleifera As An Inhibitor of Various Adipogenesis Pathways in Obesity: A Systematic Review
CP3	Yuni Retnaningtyas	The Effect of Age Difference on Coffea Canephora on Antibacterial Activity of Agnps
CP4	Viriyanata Wijaya	Alkaloids of Dicranostigma Franchetianum (Prain) Fedde and Their Inhibition of Acetyl- and Butyrylcholinesterase and Prolyloligopeptidase
CP5	Dwi Koko	Antioxidant Activities of Five Epiphytic Ferns: In vitro and insilico Molecular Docking Analysis
CP6	Nike Sari Oktavia	Breast Cancer Models In Female Rat Strain Wistar With Benzopyrene Injection

ORAL PRESENTER SCHEDULE
Saturday, November 4th 2023
Session 1 : 13.40 – 15.00

Room 1 – Ballroom (OFFLINE)
Room Topic : Pharmaceutical Research and Analytical Chemistry
Invited Speaker : Dr. apt. Valentina Yurina, S.Si, M.Si
Topic of Invited Speaker : Bacterial Live Vector as Vaccine Carrier
Moderator : apt. Luthfi Achmad M., M.Farm., S.Farm

Code	Presenter	Abstract Title
AO2	Anggita Rosiana Putri	Optimization of Ultrasound-Assisted Oil Extraction from Patin Fish (Pangasius Micronemus) with Response Surface Methodology
AO6	Bachtiar Rifai Pratita Ihsan	Determination of Curcumin Content In Curcuma Domestica Extract and Curcuma Xanthorhizza Extract By Hplc Method
AO4	Nur Atika Fatwa	Optimization of The Cryoprotectant As A Recombinant Food-Grade Lactococcus Lactis Bacteria Stabilizer For Covid-19 Vaccine Oral Formulation
AO5	Naura Salsabila Nadhifa	In Silico Studies of 3-Amino-2-Phenylquinazoline-4(3h)-One Derivate As A Potential Analgesic Against Cox-2
AO8	Rahayu Hardianti Rindiantika	Drug-Likeness Prediction and Sleep Disorder Activity Test (In Silico) Of Basil Essential Oil and Its Formulation Into Aromatherapy Derma Sticks
AO10	Roisah Nawatila	Formulation And Physical Characteristics of Hard Candy Lozenge of Citrus Limon Essential Oil On Various Types Of Sugar-Free Candy Base (Isomalt, Mannitol, Sorbitol)
AO11	Tarwadi	Preparation, Characterization, And Evaluation of Positively Charged Oligopeptides For Potential Transfection Agents

Room 2 – Ivory 1 (ONLINE)
Link Zoom : s.ub.ac.id/icsm2023 (Breakout Room 2)
Room Topic : Pharmaceutical Research and Analytical Chemistry
Invited Speaker : apt. Oktavia Eka, M.Pharm
Topic of Invited Speaker : Potential Use of Modified Starch for Drug Delivery Systems
Moderator : apt. Tamara Gusti E., M.Farm., S.Farm

Code	Presenter	Abstract Title
AO16	Taufan Hari Sugara	Anticancer Activity of Fluoroxanthone Derivatives Against HepG2 Cancer Cell Lines Based on QSAR and Molecular Docking Approaches
AO17	Nazir Ahmad	In Silico Study on Phosphodiesterase 1b Inhibition and Phytochemical Composition Of White Cabbage
AO18	Ramadhan Bagus Cahyono, S. Farm.	Jamu A, B, C, And D Antioxidant Activity and Its Relation to Total Phenolic, Flavonoids, and Alkoids Content
AO19	Asri Kusuma Wardani, S.Farm	In Vitro Anti-inflammatory Properties of Jamu X, Y, and Z via Red Blood Cells Membranes Stabilization and Protein Denaturation Inhibition
AO21	apt. Viddy Agustian Rosyidi, S.Farm., M.Sc.	Optimization of Tween 80 and Lecithin in Fennel Oil-based Nanoemulsion Containing Diclofenac Sodium
AO22	apt.Wirasti,S.Si.,M.Sc	Search for Active Compound of Brown Seaweed Padina australis Hauck As Antiaging Through Collagenase Enzyme Inhibiting

Room 3 – Ivory 3 (OFFLINE)
Room Topic **:** Clinical and Community Health Research
Invited Speaker **:** apt. Diana Lyrawati, Ph.D
Topic of Invited Speaker **:** The Chosen Antihypertensive Drugs And Their Efficacy In Blood Pressure Control In Primary Care Settings
Moderator **:** apt.Ayuk Lawuningtyas, M.Farm., S.Farm

Code	Presenter	Abstract Title
BO4	Syafira Wahyu Widowati, S.Si., M.Kes	Supplementary Zinc Consumption and Lifestyle of Young Mother During Pregnancy: A Qualitative Study Recall Experiment
BO5	Pinasti Utami	The Correlation Analysis of Moca Ina (Montreal Cognitive Assessment Ver. Indonesia) Score on The Depression Scales, Burden Levels, and Knowledges Among Dementia Caregivers
BO6	Ardaleni Frista	Validation of the Content and Application of SEPO Digital as a Measure of Pharmaceutical Care in Improving the Quality of Life of Osteoarthritis Patients.
BO7	Siti Ma'rufah	An Investigation of Patient Satisfaction In Type 2 Diabetes Mellitus with Interprofessional Collaboration Management in Developing Countries
BO8	Kawai Maharani Agustina, S.Farm.	Assessment of Parents' Knowledge Regarding the Proper Child Diarrhea Self-Medication in Malang Raya
BO9	Hening Pratiwi	Factors that related to the pharmacy students' empathy towards geriatrics: a qualitative study of educators and practitioners
BO12	Eka Kartika Untari	The Factors Affecting Ulcer Self-Care Behaviors of Foot Self-Care Prevention and Glycemic Control Among Diabetes Mellitus Patients at Type A Hospital in Yogyakarta

Room 4 – Ivory 2 (ONLINE)
Link Zoom : s.ub.ac.id/icsm2023 (Breakout Room 4)
Room Topic : Clinical and Community Health Research
Invited Speaker : Lilik Indahwati, S.ST., M.Keb
Topic of Invited Speaker : Prenatal Hypnosis To Improve Maternal Health
Moderator : Adinda Zahrani Mintarja

Code	Presenter	Abstract Title
BO17	Rara Merinda Puspitasari	The Potential Benefits Of Supplementing Vitamin D To Alleviate Depressive Symptoms: A Narrative Review
BO18	Salsabilla Firdausyiah	Financial Impact Of The Covid-19 Pandemic On Healthcare Workers: A Case Study Of Pharmacists in Healthcare Services in Yogyakarta Indonesia
BO19	Niken Larasati	Drug Related Problems and Contributing Factors Among Patients With Type 2 Dm: A Retrospective Study
BO20	apt. Kadek Ida Krisnadewi, M.Pharm.,Sci.	Implementation Of Elderly And Chronic Disease Program Activities At Community Health Centers In Indonesia
BO21	Joan Fayola	Factors Associated With Medication Non-Adherence Behavior Among Patients With Diabetes In Surabaya
BO22	apt. Noor Cahaya, M.Sc	Subjective Methods to Measure Medication Adherence In People With Schizophrenia: A Review
BO23	apt. Hilda Ema Paramita, S. Farm	Profile Antituberculosis Therapy In Tuberculosis Patients with Diabetes Mellitus

Room 5 – Ivory 4 (ONLINE)

Link Zoom : s.ub.ac.id/icsm2023 (Breakout Room 5)
Room Topic : Clinical and Community Health Research
Invited Speaker : dr. Happy Kurnia Permatasari, Ph.D
Topic of Invited Speaker : Anticancer Properties Of Caulerpa Racemosa By Altering Several Oncological Pathways
Moderator : apt. Arsy Arundina., S.Farm., MMRS

Code	Presenter	Abstract Title
BO33	Muhammad Akib Yuswar	Hypoglycemia in Geriatric Patients With Diabetes
BO34	Andrea Aprilia, dr., Sp.PK	Correlation Of Micronutrients And Cellular Immune Response After Coronavac Vaccination in Elderly People
BO35	Rasmaya Niruri	Interprofessional Approach in Pharmacogenomic: A Systematic Review.
BO36	Thareq Barasabha	Personalized 3D Printed Medicine Box Design to Enhance Medication Adherence in Pediatric Patients
CO15	Indah Tri Lestari	Influence of Red Fruit Oil on The Long-Term Hyperglycaemia Rat Model Induced By Streptozotocin
CO16	apt. Fitrawan Hernuza Pribadi, M.Sc.	Network Pharmacology on Targets And Mechanism of Hesperetin and Hesperidin In Type 2 Diabetes Mellitus
CO17	Astutiati Nurhasanah	Development of qPCR Primers For The Detection of Covid-19 – A Potential Study Tool to Demonstrating The Importance of Selecting Slowly-Evolving Gene for the Detection of Rapidly Evolving Pathogens

Room 6 – Ivory 6 (OFFLINE)

Room Topic **:** Biomolecular and Herbal Medicine

Invited Speaker **:** apt. Uswatun Khasanah, M.Farm., S.Farm

Topic of Invited Speaker **:** Development of herbal medicine from Strychnos lucida R. Br. as an antimalarial agent

Moderator **:** apt. Thia Amalia, M.Si.

Code	Presenter	Abstract Title
CO1	Dr. Muthia Rahayu Iresha, S.Si	Virtual Screening of Medicinal Plants' Bioactive Compounds to Guide Discovery of Hiv Replication Inhibitor Agents
CO2	Fami Israyusnita	The Application of Agarose Gel Electrophoresis And Quantitative Real Time Pcr to Determine Gene Copy Number In Recombinant Yeasts – An Evaluation Of Two Approaches
AO14	Rafika Sari	The Effect Of Extraction Time On The Yield And Antibacterial Activity Of Kulim (*Scorodocarpus borneensis Becc*.) Leaf And Bark Extract As An Antibacterial And Antibiofilm
CO4	Shoma Rizkifani, M.Sc., Apt	The Effect Of Acute Toxicity Test Of Red Dragon Fruit (*Hylocereus polyrhizus*) Peel Extract On Body Weight And Organ Index Of Wistar Rats Strain
CO5	apt. Robby Najini, M.Farm.	The Effect of Red Dragon Fruit (*Hylocereus polyrhizus*) Peel Tea on Human Total Cholesterol, Triglycerides, Hdl And Ldl
CO6	Yoni Rina Bintari, S.Si., M.Sc	Anti-Inflammatory Activity Of Ethanol Extract of Cananga Odorata Against Inhibition Of Bovine Serum Albumin (BSA) Denaturation
CO7	Ni Made Amelia Ratnata Dewi	Protective Effect of Sea Cucumber (*Holothuria scabra*) Extract On Inflammation In Mice

Room 7 – Ivory 5 (ONLINE)

Link Zoom : s.ub.ac.id/icsm2023 (Breakout Room 7)
Room Topic : Biomolecular and Herbal Medicine
Invited Speaker : apt. Efta Triastuti, M.Farm.Klin. Ph.D.
Topic of Invited Speaker : Cell Interaction Dynamics in Responses to a Pharmacological Treatment
Moderator : apt. Ema Pristi Yunita, M.Farm. Klin., S.Farm

Code	Presenter	Abstract Title
BO3	Riyana Noor Oktaviyanti	In-Silico Prediction of Epigallocatechin-3-Gallate (Egcg) Compare Retinol In Has 1 And Mmp 1 Target
CO9	Ayik Rosita P	Drug Discovery Screening of Artocarpus Camansi and Artocarpus Altilis Stem Bark Extracts on Mycobacterium Tuberculosis H37rv
CO10	Evi Umayah Ulfa	Production And Purification of The C-Terminal Domain of Secretory Leukocyte Protease Inhibitor
CO11	Lina Winarti	Effect Of Additional Bitter Gourd Seed Oil on The Characteristics and In Vitro Effectiveness Of Zinc Oxide Sunscreen Cream
CO12	Fifteen Aprila Fajrin	Antioxidant and Anti Hyperalgesia Activity Of Ethanol Extract And Fraction from Red Ginger (Zingiber Officinale Var. Rubrum) In Early Painful Diabetic Neuropathy Mice
CO13	Putri Dwi Apriliani	Jamu B Exhibited The Most Potential As Anti-Inflammatory Agent Compared to Jamu A, C, and D: An In Vitro Study
CO14	Ika Lailatus Sa'diah	Vey Strong and Strong Antioxidant Activity of Jamu X, Y, And Z and Its Correlation to Total Phenolic, Flavonoids, And Alkaloid Content

ORAL PRESENTER SCHEDULE
Saturday, November 4th 2023
Session 2 : 15.15 – 16.15

Room 1 – Ballroom (OFFLINE)
Room Topic **:** Pharmaceutical Research and Analytical Chemistry
Moderator **:** apt. Bachtiar R.I., M.Farm., S.Farm

Code	Presenter	Abstract Title
AO13	Reyhan Fathihah Syahri	In Silico Study of 3-Amino-7-Chloro-2-Phenylquinazolin-4(3h)-One Derivate as an Analgesic Against Cox Enzyme
AO3	Adeltrudis Adelsa Danimayostu	Determination of Vitamin D3 Loaded Self-Nanoemulsifying Drug Delivery Systems (Snedds) Based Hydrogel
AO15	Annisa Septianti Sekar Kinasih	In Silico Studies of 3-Amino-6-Chloro Quinazoline-4(3h)-One Derivates of Quinazoline as Potential Analgesics Against Cox-2 Enzyme
AO30	Ika Oktavia Wulandari	Green Synthesis And Characterization of Silver Nanoparticles Coated by Biocompatible Polymer and Its Potency in the Formulation of Sanitizer Non-Alkoholic.

Room 2 – Ivory 1 (ONLINE)
Link Zoom **:** s.ub.ac.id/icsm2023 (Breakout Room 2)
Room Topic **:** Pharmaceutical Research and Analytical Chemistry
Moderator **:** Dr. Anggita Rosiana Putri, M.Si

Code	Presenter	Abstract Title
AO23	Viviane Annisa	In Vitro-In Vivo Correlation of Beads Ketoconazole Loaded into Alginate-Gum Acacia Matrix
AO24	Normaidah	Identification of Quercetin IN 96% Ethanolic Extract of Mitragyna SPECIOSA Leaves
AO25	Lidya Ameliana	Development of Cinnamon Oil (Cinnamomum Burmanii) as An Anti-Acne Nanoemulgel and Its Effectiveness Against Propionibacterium Acnes
AO26	Rudy Salam	From Empiric to In-Silico Garlic for Anti-Diabetic: Hypothesis of Alliin as Dpp-4 Inhibitor
AO27	Yudi Wicaksono	Evaluation of Physical-Mechanical Properties of Atorvastatin Calcium-Isonicotinamide Cocrystal
AO12	Damai Ria Setyawati	Design of Liposome Formula as Gene Carrier In Hek293t Cells Using Box Behnken of Response Surface Methodology
AO31	Budipratiwi Wisudyaningsih	Optimization of Tween and Polyethylene Glycol In Diclofenac Sodium Self-Nanoemulsifying Drug Delivery System

Room 3 – Ivory 3 (OFFLINE)
Room Topic **:** Clinical and Community Health Research
Moderator **:** apt. Oktavia Eka, M.Pharm

Code	Presenter	Abstract Title
BO11	Apt. Hananditia Rachma Pramestutie., M.Farm.Klin	Pharmacists' Practice In Providing Pharmaceutical Services Related to Treating Pediatric Diarrhea In Pharmacies: A Qualitative Study
BO13	Afifah Machlaurin	Cost-Effectiveness Analysis of Adding Chest X-Ray Into Standard Rapid Test Diagnosis of Multi-Drug Resistance Tuberculosis: An Observational Study
BO15	Nur Aini Retno Hastuti	Microplastic Exposure In Adolescents Due to Daily Plastic Usage In A Clean Urban Environment: Case Study In Malang, East Java
BO16	Farroh Bintang Sabiti	The Effect of Whatsapp Reminder on Medication Adherence Among Hiv Patients In Semarang City
BO37	Yuseva Sariati	Implementation of Reproductive Health Education and Maternal Role Attainment on The Quality of Life of Adolescent Mothers
BO10	Tamara Gusti Ebtavanny	The Relationship of Parents' Knowledge and Attitudes Regarding Childhood Diarrhea Treatment

Room 4 – Ivory 2 (ONLINE)
Link Zoom **:** s.ub.ac.id/icsm2023 (Breakout Room 4)
Room Topic **:** Clinical and Community Health Research
Invited Speaker **:** Fatmawati, M.keb. S.Keb
Topic of Invited Speaker : Advancing Midwifery Education Through Telehealth
Moderator **:** Niken Setyaningrum

Code	Presenter	Abstract Title
BO24	Intan Puspita Sari	Implementation of Antibiotic Stewardship Program In Hospitalised Children: A Systematic Review
BO25	Difa Intannia	The Role of Health Workers from The Perspective of Pharmacist Professional Education Students
BO26	Bezaleel Yehuda Antonio	Public's Knowledge of Tuberculosis Disease, Management And Prevention – Findings from A Systematic Review
BO27	Iqhro' Samudro Thirto Buono	The Applicability of Different Classification Systems to Identify Drug Related Problems In Tuberculosis Patients
BO28	Radhwa Fauztina	Cost-Effectiveness Analysis of The Combination of Amlodipine And Candesartan Compared to Furosemide And Candesartan on Chronic Kidney Disease Outpatients with Hypertension in Yogyakarta Indonesia
BO38	Nisa Febrinasari	Need Assessment of Indonesian Community Pharmacists in Mental Health Training: A Qualitative Study

Room 5 – Ivory 4 (ONLINE)

Link Zoom : s.ub.ac.id/icsm2023 (Breakout Room 5)
Room Topic : Clinical and Community Health Research
Moderator : Dr. apt. Valentina Yurina, M.Si

Code	Presenter	Abstract Title
CO18	Zulkarnain	Evaluating The Potency of Active Compounds from Patchouli Oil (Pogostemon Cablin Benth.) as Wound Healing Activation Candidate through The Inhibition of GSK-3β and Collagenase Enzyme
BO30	Shafira Billah Ariani Wahyudi	Knowledge, Attitude, and Practice Towards Hepatitis B Vaccine Among Students: A Scoping Review
BO31	Herningtyas Nautika Lingga	Evaluation of Drug Management at Pangeran Jaya Sumitra Hospital, Kotabaru Regency
BO14	Ibnu Agus Ariyanto	Unique Cell Population Cell Discovery Pipeline Successfully Identify Difference of Vδ2 + / Vδ2 - Γδ T-Cells In HIV Patients with Healthy Subjects Using Unsupervised Machine Learning Analysis, The Markers Of Cardiovascular Risk In Hiv Patients
BO29	Chilmia Nurul Fatiha	Indonesian Pharmacist Intervention to Improve Medication Adherence Among Hypertensive Patients: Systematic Review
AO1	Bismi Yasinta Maharani	Preparation, Characterization, and In Vitro Evaluation of Low Molecular Weight Branched Polyethyleneimine 800 Da (Bpei-800)-Based Liposomes as Transfection Agents

Room 6 – Ivory 6 (OFFLINE)

Room Topic : Biomolecular and Herbal Medicine
Moderator : apt. Queen Intan Nurrahmah., Ph.D

Code	Presenter	Abstract Title
AO7	Dyahati Wahyurini, Md	The Antidiabetic Potency of Ficus Deltoidea Jack: A Computational Analysis of Its Biological and Pharmacological Bioactive Compounds
AO9	Berliana Dwi Novita	Drug-Likeness Prediction and Anti-Anxiety Activity Test (In Silico) of Star Anise Essential Oil and Its Formulation Into Aromatherapy Cream
CO3	Desti Putri Rahmadani	Exploration Of Antibacterial And Antioxidant Activity of Foeniculum Vulgare Mill.

Room 7 – Ivory 5 (ONLINE)

Link Zoom **:** s.ub.ac.id/icsm2023 (Breakout Room 7)

Room Topic **:** Biomolecular and Herbal Medicine

Moderator **:** apt. Uswatun Khasanah, M.Farm., S.Farm

Code	Presenter	Abstract Title
CO8	Syarifah Raisha Muhayya	Sars-Cov-2 Multi-Epitope Subunit Vaccine Proof-Of-Concept from The In Silico Study with Protein Expression in E. Coli Bl21
BO1	Meilina Kharisma Fortuna Dewi S,Farm	Detection of Paracetamol Medicinal Chemicals in Sciatica Herbs Using Near-Infrared Spectroscopy And Chemometric
BO2	Rizka Nurullita Octavia, S.Farm	Detection of Mefenamic Acid Medicinal Chemicals in Sciatica Herbs Using Near-Infrared Spectroscopy And Chemometric
BO32	Siti Muslichah	Herbal Ingredients of Macan Kerah: Composition, How To Use, and Impact on The Health of Banyuwangi Osing People, East Java Indonesia
AO29	Fatmaria	The Application Effectiveness Antibacterial of Hand Sanitizer With Rattan Latung (Daemonorops Fissus (Miq.) Blume) Extract
AO28	Annisa Maghfira	In-Silico Analysis of Brassica Oleraceae Bioactive Compounds Against Alzheimer's Disease by Targeting Acetylcholinesterase
CO19	Dewi Dianasari	The Effect of The Extraction Methods of Apu-Apu Herbs (Pistia Stratiotes) on Antioxidant Activity And Identification of Its Active Compounds

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